TEXAS A&M UNIVERSITY

CSCE 421: Machine Learning

Lecture 5

Overview

- Linear Regression: What have we learnt so far
    - Representation
    - Analytic Solution: Ordinary Least Squares
- Linear Regression: Numerical solution
    - General gradient descent
    - Gradient descent for linear regression (batch, stochastic, mini-batch)
- Non-linear basis function for regression

Overview

- Linear Regression Basics
  - Representation
  - Analytic Solution: Ordinary Least Squares
- Linear Regression: Numerical solution
  - General gradient descent
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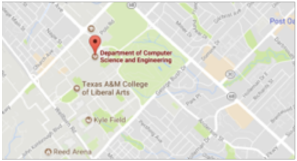
Linear Regression: Example



Apartment Amenities

Pet Policy

Dogs Allowed: Breed Restrictions May Apply.

- $250 Fee
- 2 Pet Limit

Cats Allowed

- $250 Fee
- 2 Pet Limit

Fitness & Recreation

- Fitness Center
- Pool
- Volleyball Court

Living Space

- Carpet
- Attic
- Crown Molding
- Views
- Walk-In Closets

Outdoor Space

- Balcony
- Patio
- Porch
- Yard
- Barbecue Area
- Barbecue/Grill

Parking

Surface Lot

6 spaces; Assigned Parking.

Services

- Maintenance on site
- Property Manager on Site
- Bilingual
- Courtesy Patrol
- Trash Pickup - Curbside
- Recycling
- Planned Social Activities
- Pet Play Area

Kitchen

- Dishwasher
- Disposal
- Ice Maker
- Granite Countertops
- Kitchen
- Microwave
- Oven
- Refrigerator
- Freezer
- Instant Hot Water

Property Information

- Built in 2015
- 442 Units/2 Stories

Lease Length

August 1 - July 22

Outdoor Space

- Grill
- Waterfront
- Pond

Features

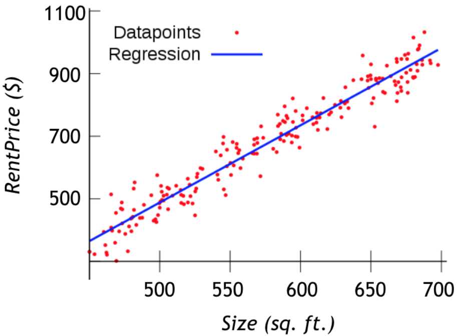
- High Speed Internet Access
- Washer/Dryer
- Air Conditioning
- Heating
- Ceiling Fans
- Smoke Free
- Cable Ready
- Tub/Shower
- Framed Mirrors

Source: apartments.com

$$RentPrice = w_0 + w_1 \times Size + w_2 \times DistanceFromCS + \ldots$$

Linear Regression: Example

$$RentPrice = w_0 + w_1 \times Size + w_2 \times DistanceFromCS + \ldots$$



Linear Regression: Example

- Input $\mathbf{x}$: apartment attributes (e.g., size, neighborhood)
- Output y: rent price of apartment
- Model parameters $\mathbf{w}$
- Linear model: $y = f(\mathbf{x}|\mathbf{w}) = \mathbf{w}^T\mathbf{x} = w_1 x + 1 + \ldots + w_D x_D$
- Non-linear model: $y = f(\mathbf{x}|\mathbf{w}) = \mathbf{w}^T\phi(\mathbf{x})$

Linear Regression: Example

$$RentPrice = w_0 + w_1 \times Size + w_2 \times DistanceFromCS + \ldots$$

$$\mathrm{RentPrice} = w_0 + w_1 \times \mathrm{Size} + w_2 \times \mathrm{DistanceFromCS} + \ldots$$

How do we find the unknown model parameters $\{w_0, w_1, w_2, \ldots\}$?

We use training data!

Training Sample	Size (sq.ft.)	DistanceFromCS (miles)	RentPrice ($)
1	498	11.9	675
2	513	8.6	750
3	621	8.3	800
4	710	3.4	965
...	...	...	...

Linear Regression

- **Representation:** linear combination of features

  $f : \mathbf{x} \rightarrow y, \;\; f(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$
- **Evaluation**: Minimizing the residual sum of squares

  $\min_{\mathbf{w}} RSS(\mathbf{w}), \;\; RSS(\mathbf{w}) = (\mathbf{y} - \mathbf{X}\mathbf{w})^T(\mathbf{y} - \mathbf{X}\mathbf{w})$
- **Optimization**: Analytical $\rightarrow$ Ordinary least squares (OLS) solution

  $\mathbf{w}^* = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$

  Is this a global minimum? $\rightarrow$ 2nd derivative test

Linear Regression: Global minimum

Theorem

Consider an optimization problem

$$\min f(\mathbf{x}) \;\; \text{s.t.} \;\; \mathbf{x} \in \Omega$$

where f is a convex function and Ω is a convex set.

Then any **local** minimum is also a **global** minimum.

How do we find in f is convex?

Linear Regression: Global minimum

Definition 1

A set Ω is convex if for all $x, y \in \Omega$ and for all $\lambda \in [0,1]$

$$\lambda x + (1-\lambda)y \in \Omega$$

[In practice, if we draw a line between any two points of the set, every point on the line still lies within this set]

convex non-convex

Linear Regression: Global minimum

Definition 2

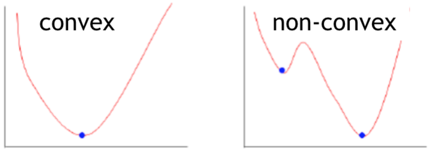
A function f is convex if its domain $\mathrm{dom}(f)$ is a convex set and for all $x, y \in \mathrm{dom}(f)$ and $\lambda \in [0,1]$

$$f(\lambda x + (1-\lambda)y) \leq \lambda f(x) + (1-\lambda) f(y)$$

[In practice, the line segment connecting $(x, f(x))$ and $(y, f(y))$ should sit above the graph]

The second-derivative test

If the Hessian matrix $\mathbf{H_f}$ of f is positive semi-definite, then f is convex.
i.e. $\mathbf{u}^T \mathbf{H_f} \mathbf{u} \geq 0 \; , \;\; \forall \mathbf{u}$



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Linear Regression: Computational Complexity

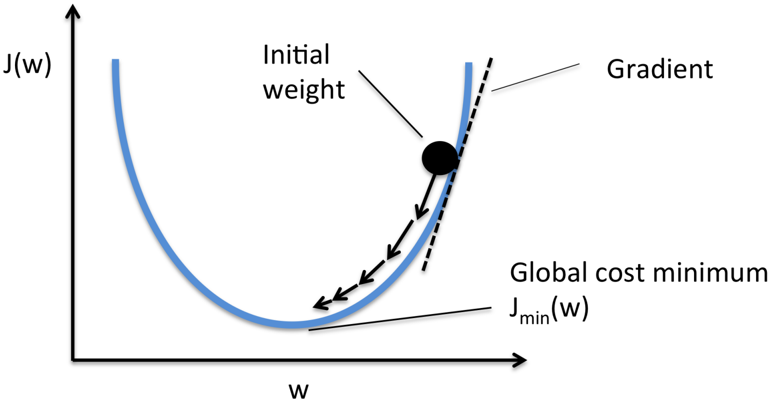
- Bottleneck for computing the solution $\mathbf{w}^* = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$ is to invert the matrix $\mathbf{X}^T\mathbf{X} \in \mathbb{R}^{D\times D}$
- Computational complexity is $O((D+1)^3)$ using Gauss-Jordan elimination
    - Impractical for large D
- Alternative
    - Find approximate solution through an iterative optimization algorithm
    - e.g. Gradient Descent

Gradient Descent

- Iterative algorithm finding a function's minimum via local search
- Standard optimization algorithm in many ML applications
  - e.g. linear regression, logistic regression
  - scales well to large datasets (e.g. no matrix multiplication)
  - proof that it solves many convex problems
  - good heuristic to non-convex problems as well
- **Input:** Function $J(\mathbf{w}) \in \mathbb{R}$
- **Output:** Local minimum $\mathbf{w}^*$
- **Goal:** Minimize $J(\mathbf{w})$ via greedy local search

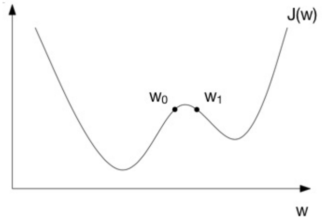
Gradient Descent

1-dimensional example: $J(w) = w^2$



Gradient Descent: 1-dimensional case

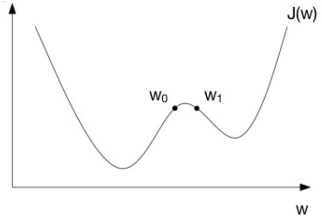
What will happen if we try to minimize $J(w)$ via a local search?



- Starting from w_0
  - We look to the right ($J(w) \uparrow$) and to the left ($J(w) \downarrow$)
  - We take a small step to the left
  - We repeat the above until we reach the left basin
- Starting from w_1
  - We similarly reach the right basin
- It is clear that the outcome depends on the starting point

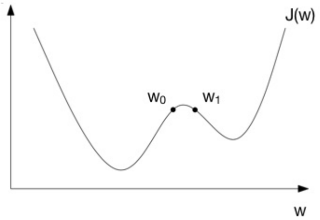
Gradient Descent: 1-dimensional case

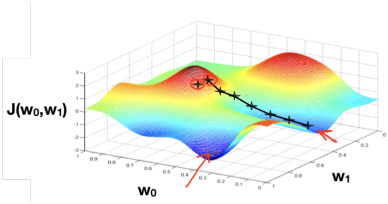
More formally, we do the following



- While $J'(w) \neq 0$
  - If $J'(w) > 0$ (i.e. $J(w) \uparrow$), move w a little bit to the left
  - If $J'(w) < 0$ (i.e. $J(w) \downarrow$), move w a little bit to the right
- The derivative $J'(w)$ is used to decide which direction to move
- In other words, move w towards the direction of $-J'(w)$

Gradient Descent: Algorithm Outline





[Source: Machine Learning, Coursera, Andrew Ng]

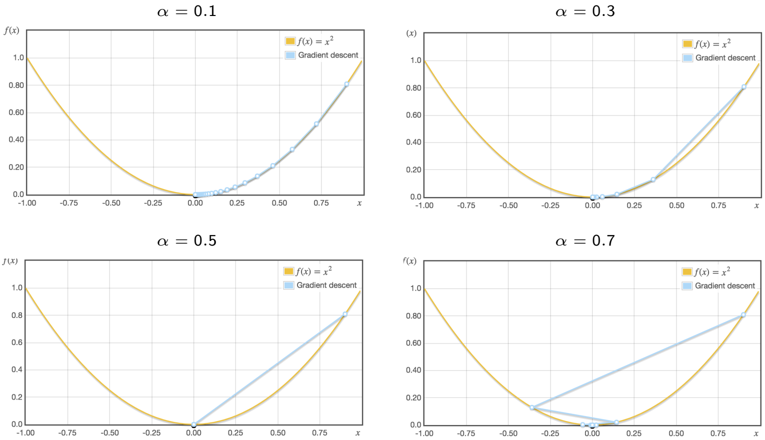
1-dimensional

1. Initialize w, ϵ, $\alpha(\cdot)$, $k := 0$
2. While $\left|\frac{dJ(w)}{dw}\right| > \epsilon$
   - 2a $k := k + 1$
   - 2b $w := w - \alpha(k) \cdot \frac{dJ(w)}{dw}$

d-dimensional

1. Initialize $\mathbf{w}$, ϵ, $\alpha(\cdot)$, $k := 0$
2. While $\|\nabla J(\mathbf{w})\|_2 > \epsilon$
   - 2a $k := k + 1$
   - 2b $\mathbf{w} := \mathbf{w} - \alpha(k) \cdot \nabla J(\mathbf{w})$

Gradient Descent: Step size (or learning rate) α



- If $\alpha(k)$ too small, convergence is unnecessarily slow
- If $\alpha(k)$ too large, correction process will overshoot and can diverge

Source: `http://www.onmyphd.com/?p=gradient.descent`

Gradient Descent: Step size (or learning rate) α

How to chose α?

- In practice, through experimentation
  - Check how $J(\mathbf{w})$ behaves over iterations for multiple α
  - α is a hyper-parameter
  - Therefore it can be tuned using a dev-set or a cross-validation framework

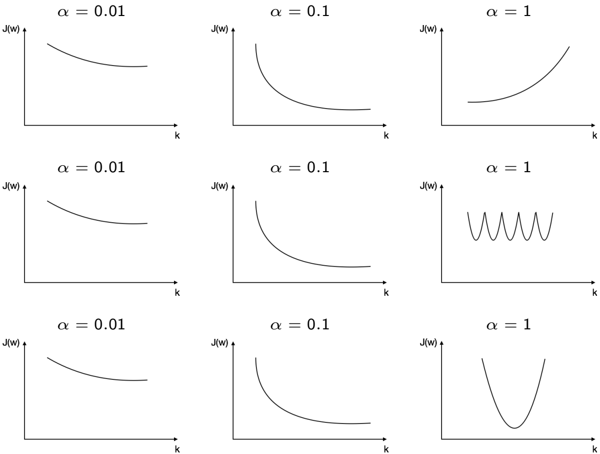
Gradient Descent: Step size (or learning rate) α

Question: A cost function $J(\mathbf{w})$ is optimized with Gradient Descent (GD) using different step size values α. We plot $J(\mathbf{w})$ w.r.t. the number of GD iterations k. Which of the following graph triplets can hold?

A

B

C

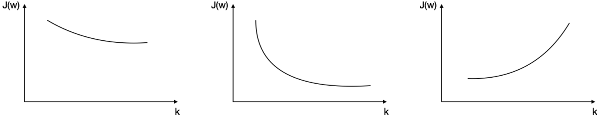


Gradient Descent: Step size (or learning rate) α

Question: A cost function $J(\mathbf{w})$ is optimized with Gradient Descent (GD) using different step size values α. We plot $J(\mathbf{w})$ w.r.t. the number of GD iterations k. Which of the following graph triplets can hold?

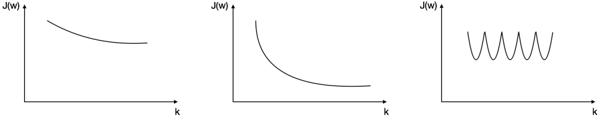
A

$\alpha = 0.01$ | $\alpha = 0.1$ | $\alpha = 1$



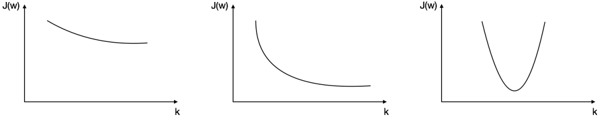
B

$\alpha = 0.01$ | $\alpha = 0.1$ | $\alpha = 1$



C

$\alpha = 0.01$ | $\alpha = 0.1$ | $\alpha = 1$



All answers can occur.

Gradient Descent: Stopping rule

- Hyper-parameter ϵ (i.e. $\|\nabla J(\mathbf{w})\|_2 > \epsilon$) determines when to stop
- Small ϵ: many iterations but higher quality solution
- Large ϵ: less iterations with the cost of more approximate solution
- How to chose ϵ in practice?
  - Try various values to achieve balance between cost and precision
  - Again use some type of cross-validation framework

- Hyperparameters: Parameters set before the beginning of the learning process (e.g. α, ϵ in gradient descent)
- Hyperparameter tuning: The process of choosing a set of optimal hyperparameters for the learning process
- Model parameters: The parameters learned during the learning process (e.g. weights $\mathbf{w}$ in linear regression)

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Gradient Descent in Linear Regression

We can now derive the algorithm outline for minimizing the residual square sum (RSS) error of linear regression with gradient descent

- The residual sum of squares is the cost function:
$$\begin{aligned} J(\mathbf{w}) = RSS(\mathbf{w}) &= (\mathbf{y} - \mathbf{X}\mathbf{w})^T(\mathbf{y} - \mathbf{X}\mathbf{w}) \\ &= \mathbf{y}^T\mathbf{y} - 2(\mathbf{X}\mathbf{w})^T\mathbf{y} + (\mathbf{X}\mathbf{w})^T(\mathbf{X}\mathbf{w}) \\ &= \mathbf{y}^T\mathbf{y} - 2\mathbf{w}^T(\mathbf{X}^T\mathbf{y}) + \mathbf{w}^T(\mathbf{X}^T\mathbf{X})\mathbf{w} \end{aligned}$$
- Gradient Descent optimization expression:
$$\mathbf{w} := \mathbf{w} - \alpha(k) \cdot \nabla J(\mathbf{w})$$
$$\nabla J(\mathbf{w}) = \frac{\vartheta RSS(\mathbf{w})}{\vartheta \mathbf{w}} = -2\mathbf{X}^T\mathbf{y} + 2\mathbf{X}^T\mathbf{X}\mathbf{w} = 0$$

Gradient Descent in Linear Regression

Question: Derive the algorithm outline for minimizing the residual square sum (RSS) error of linear regression with gradient descent

(Batch) Gradient Descent for Linear Regression

1 Initialize $\mathbf{w}$, ϵ, $\alpha(\cdot)$, $k := 0$

2 While $\|\nabla RSS(\mathbf{w})\|_2 > \epsilon$

  2a $k := k + 1$

  2b $\mathbf{w} := \mathbf{w} - \alpha(k) \cdot \left(\mathbf{X}^T \mathbf{X} \mathbf{w} - \mathbf{X}^T \mathbf{y}\right)$

Gradient Descent in Linear Regression

Stochastic Gradient Descent for Linear Regression

Update weights using one sample at a time

1. Initialize $\mathbf{w}$, ϵ, $\alpha(\cdot)$, $k := 0$
2. Loop until convergence
   - 2a $k := k + 1$
   - 2b Randomly choose a sample $(\mathbf{x_i}, y_i)$
   - 2c Compute its contribution to the gradient $\mathbf{g_i} = (\mathbf{x_i}^T \mathbf{w} - y_i) \cdot \mathbf{x_i}$
   - 2d Update the weights $\mathbf{w} := \mathbf{w} - \alpha(k) \cdot \mathbf{g_i}$

Gradient Descent in Linear Regression

Mini-Batch Gradient Descent for Linear Regression

Update weights using subset of samples at a time

1 Initialize $\mathbf{w}$, ϵ, $\alpha(\cdot)$, $k := 0$

2 Loop until convergence

   2a $k := k + 1$

   2b Randomly choose a subset of samples $S = \{(\mathbf{x_i}, y_i), \ldots, (\mathbf{x_{i+M}}, y_{i+M})\}$

   2c Form the mini-batch data matrix $\mathbf{X_S} = \begin{bmatrix} \mathbf{x_i}^T \\ \vdots \\ \mathbf{x}_{\mathbf{i+M}}^T \end{bmatrix}$

   2d Update the weights $\mathbf{w} := \mathbf{w} - \alpha(k) \cdot \left(\mathbf{X_S}^T \mathbf{X_S} \mathbf{w} - \mathbf{X_S}^T \mathbf{y} \right)$

- Good compromise between batch and stochastic gradient descent
- Common mini-batch sizes range between M=50-250 samples

Gradient Descent in Linear Regression

- Batch gradient descent computes exact gradient
- Stochastic gradient descent
  - Computes approximate gradient using one sample per iteration
  - Its expectation equals the true gradient
- Mini-batch gradient descent
  - Computes gradient based on subset of samples
- For large-scale problems stochastic or mini-batch descent often work well

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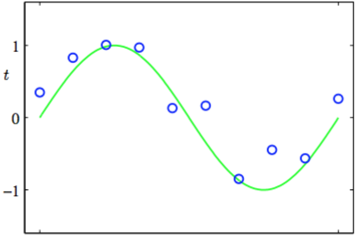
What if data does not fit a line?

Example: Samples from a sine function



We can use a non-linear basis function
$\phi(\mathbf{x}) : \mathbf{x} \in \mathbb{R}^D \rightarrow \mathbf{z} \in \mathbb{R}^M$

We can apply our linear regression model to the new features
$y_i = \mathbf{w}^T \mathbf{z_i} = \mathbf{w}^T \phi(\mathbf{x_i})$
$RSS(\mathbf{w}) = \sum_{n=1}^{N} \left(y_i - \mathbf{w}^T \phi(\mathbf{x_i})\right)^2, \ \mathbf{w} \in \mathbb{R}^M$
Example: $\mathbf{x} = [x_1, x_2]^T \in \mathbb{R}^2$, $\phi(\mathbf{x}) = [x_1, x_2^2, x_1^3 + x_2]^T \in \mathbb{R}^3$

Non-Linear Basis Function

Residual sum of squares

$$RSS(\mathbf{w}) = \sum_{n=1}^{N} \left(y_i - \mathbf{w}^T \phi(\mathbf{x_i})\right)^2 = (\mathbf{y} - \boldsymbol{\Phi}\mathbf{w})^T(\mathbf{y} - \boldsymbol{\Phi}\mathbf{w})$$

Non-linear design matrix

$$\boldsymbol{\Phi} = \begin{bmatrix} \phi(\mathbf{x_1})^T \\ \phi(\mathbf{x_2})^T \\ \vdots \\ \phi(\mathbf{x_N})^T \end{bmatrix} \in \mathbb{R}^{N \times M}$$

LMS solution with the non-linear design matrix

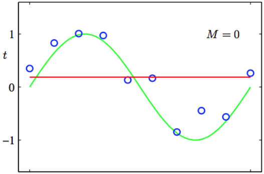
$$\mathbf{w}^{LMS} = (\boldsymbol{\Phi}^T\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^T\mathbf{y}$$

Non-Linear Basis Function

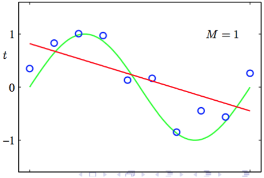
Example: Samples from a sine function

Polynomial basis function $\phi(\mathbf{x}) = [1\ x\ \ldots\ x^M]^T$

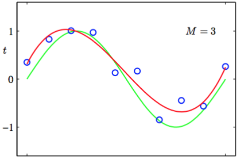
$M = 0$ underfitting



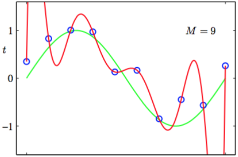
$M = 1$ underfitting



$M = 3$



$M = 9$ overfitting



Overfitting

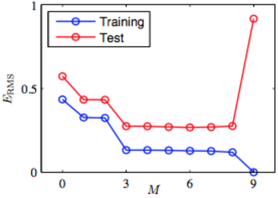
Weights of high order polynomials are very large

$$y_i = \mathbf{w}^T \mathbf{z_i} = \mathbf{w}^T \phi(\mathbf{x_i}), \quad \mathbf{z_i} = \phi(\mathbf{x_i}) \in \mathbb{R}^M$$

	$M = 0$	$M = 1$	$M = 3$	$M = 9$
w_0	0.19	0.82	0.31	0.35
w_1		-1.27	7.99	232.37
w_2			-25.43	-5321.83
w_3			17.37	48568.31
w_4				-231639.30
w_5				640042.26
w_6				-1061800.52
w_7				1042400.18
w_8				-557682.99
w_9				125201.43

Overfitting

- The risk of using highly flexible (complicated) models without enough data
- Leads to poor generalization
- How to detect overfitting?
  - Plot model complexity (e.g. polynomial order) versus objective function
  - As complexity increases, performance on training improves, while on testing first improves and then deteriorates
- How to avoid overfitting?
  - More data or regularization



Linear Regression: To summarize

- **Representation:** linear and non-linear basis

$$f: \mathbf{x} \to y, \quad f(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$$
$$f: \mathbf{z} \to y, \quad f(\mathbf{x}) = \mathbf{w}^T\mathbf{z} = \mathbf{w}^T\phi(\mathbf{x}), \quad \phi: \mathbf{x} \in \mathbb{R}^D \to \mathbf{z} \in \mathbb{R}^M$$

- **Evaluation**: Minimizing residual sum of squares

$$\min_{\mathbf{w}} RSS(\mathbf{w}), \quad RSS(\mathbf{w}) = (\mathbf{y} - \mathbf{X}\mathbf{w})^T(\mathbf{y} - \mathbf{X}\mathbf{w})$$
$$\min_{\mathbf{w}} RSS(\mathbf{w}), \quad RSS(\mathbf{w}) = (\mathbf{y} - \boldsymbol{\Phi}\mathbf{w})^T(\mathbf{y} - \boldsymbol{\Phi}\mathbf{w})$$

- **Analytic Optimization**: Ordinary least squares (OLS) solution

$$\mathbf{w}^* = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}, \quad \mathbf{w}^* = (\boldsymbol{\Phi}^T\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^T\mathbf{y}$$

- **Approximate Optimization**: Gradient descent
- **Readings:** Alpaydin Ch 2, Abu-Mostafa Ch 3.2; Handouts 6,7 on Piazza
- **Code example:** *GradientDescentExample.ipynb* on Google Drive
`https://colab.research.google.com/drive/1msq7fZ4Z88MIr6qaJStfEgsYMQ40sy3R`